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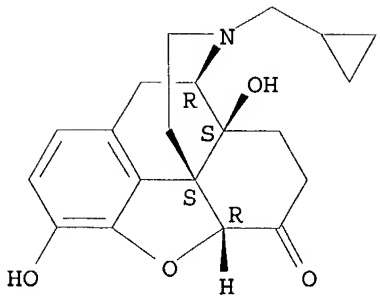
L2 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 16590-41-3 REGISTRY
ED Entered STN: 16 Nov 1984
CN Morphinan-6-one, 17-(cyclopropylmethyl)-4,5-epoxy-3,14-dihydroxy-, (5α)- (9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Morphinan-6-one, 17-(cyclopropylmethyl)-4,5α-epoxy-3,14-dihydroxy- (8CI)
OTHER NAMES:
CN 1-N-Cyclopropylmethyl-7,8-dihydro-14-hydroxynormorphinone
CN Depotrex
CN EN 1639
CN N-Cyclopropylmethylnoroxymorphone
CN Naltrel
CN **Naltrexone**
CN Nemexin
CN ReVia
CN UM 792
FS STEREOSEARCH
MF C20 H23 N O4
CI COM
LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAPLUS, CASREACT, CBNB, CEN, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, DDFU, DIOGENES, DRUGU, EMBASE, HSDB*, IFICDB, IFIPAT, IFIUDB, IMSDRUGNEWS, IMSPATENTS, IMSRESEARCH, IPA, MEDLINE, MRCK*, NIOSHTIC, PHAR, PROMT, PROUSDDR, PS, RTECS*, SPECINFO, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL, VETU
(*File contains numerically searchable property data)
Other Sources: EINECS**, WHO
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Book; Conference; Dissertation; Journal; Patent; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); MSC (Miscellaneous); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C3	C3	3	C3	1.13.1	1
C4O-C5N-C6-C6-C6	OC4-NC5-C6-C6-C6	5-6-6-6-6	C16NO	4766.1.4	1

Absolute stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	1	pH 4	(1) ACD
Bioconc. Factor (BCF)	5.20	pH 7	(1) ACD
Bioconc. Factor (BCF)	14.0	pH 8	(1) ACD
Bioconc. Factor (BCF)	3.63	pH 10	(1) ACD
Boiling Point (BP)	558.1+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	88.40+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	291.4+/-54.2 deg C		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	2		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD
Koc (KOC)	1	pH 4	(1) ACD
Koc (KOC)	79.0	pH 7	(1) ACD
Koc (KOC)	214	pH 8	(1) ACD
Koc (KOC)	55.3	pH 10	(1) ACD
logD (LOGD)	-1.13	pH 1	(1) ACD
logD (LOGD)	-0.96	pH 4	(1) ACD
logD (LOGD)	1.42	pH 7	(1) ACD
logD (LOGD)	1.85	pH 8	(1) ACD
logD (LOGD)	1.26	pH 10	(1) ACD
logP (LOGP)	1.966+/-0.564		(1) ACD
Molar Solubility (SLB.MOL)	>=0.1 - <1 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	>=0.1 - <1 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	341.40 ⇐ 1 mmole.		(1) ACD
pKa (PKA)	9.39+/-0.60	Most Acidic	(1) ACD
pKa (PKA)	7.40+/-0.40	Most Basic	(1) ACD
Vapor Pressure (VP)	2.71E-13 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.67 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

1763 REFERENCES IN FILE CA (1907 TO DATE)
43 REFERENCES TO NON-SPECIF

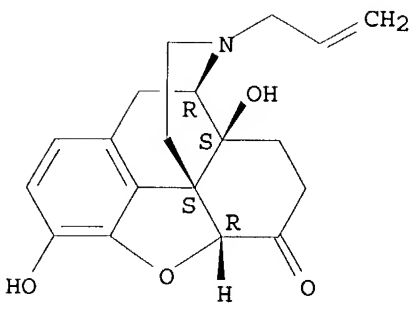
6. 100μ mole.

L3 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 465-65-6 REGISTRY
ED Entered STN: 16 Nov 1984
CN Morphinan-6-one, 4,5-epoxy-3,14-dihydroxy-17-(2-propenyl)-, (5α)-
(9CI) (CA INDEX NAME)
OTHER CA INDEX NAMES:
CN Morphinan-6-one, 17-allyl-4,5α-epoxy-3,14-dihydroxy- (8CI)
CN Normorphinone, N-allyl-7,8-dihydro-14-hydroxy- (7CI)
OTHER NAMES:
CN (-)-Naloxone
CN 12-Allyl-7,7a,8,9-tetrahydro-3,7a-dihydroxy-4aH-8,9c-
iminoethanophenanthro[4,5-bcd]furan-5(6H)-one
CN l-Naloxone
CN **Naloxone**
CN NSC 70413
FS STEREOSEARCH
DR 5592-87-0
MF C19 H21 N O4
CI COM
LC STN Files: ADISNEWS, AGRICOLA, ANABSTR, AQUIRE, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CABA, CANCERLIT, CAOLD, CAPLUS, CASREACT, CBNB, CEN, CHEMINFORMRX, CHEMLIST, CIN, CSCHEM, DDFU, DIOGENES, DRUGU, EMBASE, HSDB*, IFICDB, IFIPAT, IFIUDB, IMSCOSEARCH, IPA, MEDLINE, MRCK*, NIOSHTIC, PHAR, PROMT, PROUSDDR, PS, RTECS*, SPECINFO, TOXCENTER, USAN, USPAT2, USPATFULL, VETU
(*File contains numerically searchable property data)
Other Sources: EINECS**, WHO
(**Enter CHEMLIST File for up-to-date regulatory information)
DT.CA CAplus document type: Conference; Dissertation; Journal; Patent; Report
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); PREP (Preparation); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses); NORL (No role in record)
RLD.NP Roles for non-specific derivatives from non-patents: ANST (Analytical study); BIOL (Biological study); FORM (Formation, nonpreparative); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C4O-C5N-C6-C6-C6	OC4-NC5-C6-C6-C6	5-6-6-6-6	C16NO	4766.1.4	1

Absolute stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	1	pH 4	(1) ACD
Bioconc. Factor (BCF)	11.9	pH 7	(1) ACD
Bioconc. Factor (BCF)	15.6	pH 8	(1) ACD
Bioconc. Factor (BCF)	3.30	pH 10	(1) ACD
Boiling Point (BP)	532.8+/-50.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	85.12+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	276.1+/-54.2 deg C		(1) ACD
H acceptors (HAC)	5		(1) ACD
H donors (HD)	2		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD
Koc (KOC)	1	pH 4	(1) ACD
Koc (KOC)	186	pH 7	(1) ACD
Koc (KOC)	242	pH 8	(1) ACD
Koc (KOC)	51.4	pH 10	(1) ACD
logD (LOGD)	-1.18	pH 1	(1) ACD
logD (LOGD)	-0.57	pH 4	(1) ACD
logD (LOGD)	1.77	pH 7	(1) ACD
logD (LOGD)	1.88	pH 8	(1) ACD
logD (LOGD)	1.21	pH 10	(1) ACD
logP (LOGP)	1.918+/-0.582		(1) ACD
Molar Solubility (SLB.MOL)	>=0.1 - <1 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	>=0.1 - <1 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	327.37		(1) ACD
pKa (PKA)	9.38+/-0.60	Most Acidic	(1) ACD
pKa (PKA)	6.61+/-0.40	Most Basic	(1) ACD
Vapor Pressure (VP)	3.49E-12 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software Solaris V4.67 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

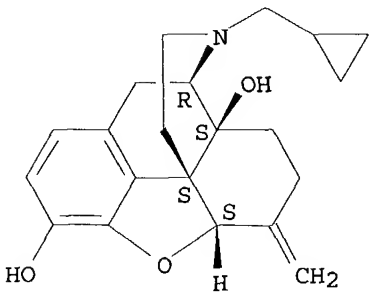
5000 REFERENCES IN FILE CA (1907 TO DATE)
28 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
5009 REFERENCES IN FILE CAPLUS (1907 TO DATE)
10 REFERENCES IN FILE CAOLD (PRIOR TO 1967)

L4 ANSWER 1 OF 1 REGISTRY COPYRIGHT 2004 ACS on STN
RN 55096-26-9 REGISTRY
ED Entered STN: 16 Nov 1984
CN Morphinan-3,14-diol, 17-(cyclopropylmethyl)-4,5-epoxy-6-methylene-, (5α)- (9CI) (CA INDEX NAME)
OTHER NAMES:
CN (-)-Nalmefene
CN 6-Deoxo-6-methylenenaltrexone
CN 6-Desoxy-6-methylenenaltrexone
CN JF 1
CN **Nalmefene**
CN Nalmetrene
CN ORF 11676
FS STEREOSEARCH
MF C21 H25 N O3
CI COM
LC STN Files: ADISINSIGHT, ADISNEWS, AGRICOLA, ANABSTR, BEILSTEIN*, BIOBUSINESS, BIOSIS, BIOTECHNO, CA, CANCERLIT, CAPLUS, CBNB, CHEMCATS, CIN, CSCHEM, DDFU, DIOGENES, DRUGU, EMBASE, HSDB*, IMSDRUGNEWS, IMSPATENTS, IMSRESEARCH, IPA, MEDLINE, MRCK*, PHAR, PROMT, PROUSDDR, PS, RTECS*, SYNTHLINE, TOXCENTER, USAN, USPAT2, USPATFULL, VETU
(*File contains numerically searchable property data)
Other Sources: WHO
DT.CA CAplus document type: Dissertation; Journal; Patent
RL.P Roles from patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); RACT (Reactant or reagent); USES (Uses)
RLD.P Roles for non-specific derivatives from patents: BIOL (Biological study); USES (Uses)
RL.NP Roles from non-patents: ANST (Analytical study); BIOL (Biological study); PREP (Preparation); PROC (Process); PRP (Properties); USES (Uses)

Ring System Data

Elemental Analysis EA	Elemental Sequence ES	Size of the Rings SZ	Ring System Formula RF	Ring Identifier RID	RID Occurrence Count
C3	C3	3	C3	1.13.1	1
C4O-C5N-C6-C6-C6	OC4-NC5-C6-C6-C6	5-6-6-6-6	C16NO	4766.1.4	1

Absolute stereochemistry.



Calculated Properties (CALC)

PROPERTY (CODE)	VALUE	CONDITION	NOTE
Bioconc. Factor (BCF)	1	pH 1	(1) ACD
Bioconc. Factor (BCF)	1	pH 4	(1) ACD
Bioconc. Factor (BCF)	17.8	pH 7	(1) ACD
Bioconc. Factor (BCF)	58.8	pH 8	(1) ACD
Bioconc. Factor (BCF)	23.6	pH 10	(1) ACD
Boiling Point (BP)	507.9+/-45.0 deg C	760.0 Torr	(1) ACD
Enthalpy of Vap. (HVAP)	81.93+/-3.0 kJ/mol		(1) ACD
Flash Point (FP)	261.0+/-51.7 deg C		(1) ACD
H acceptors (HAC)	4		(1) ACD
H donors (HD)	2		(1) ACD
Koc (KOC)	1	pH 1	(1) ACD
Koc (KOC)	1	pH 4	(1) ACD
Koc (KOC)	177	pH 7	(1) ACD
Koc (KOC)	584	pH 8	(1) ACD
Koc (KOC)	234	pH 10	(1) ACD
logD (LOGD)	-0.28	pH 1	(1) ACD
logD (LOGD)	-0.15	pH 4	(1) ACD
logD (LOGD)	2.16	pH 7	(1) ACD
logD (LOGD)	2.68	pH 8	(1) ACD
logD (LOGD)	2.28	pH 10	(1) ACD
logP (LOGP)	2.824+/-0.507		(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 1	(1) ACD
Molar Solubility (SLB.MOL)	>=0.01 - <0.1 mol/L	pH 4	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 7	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 8	(1) ACD
Molar Solubility (SLB.MOL)	<0.01 mol/L	pH 10	(1) ACD
Molecular Weight (MW)	339.43		(1) ACD
pKa (PKA)	9.61+/-0.60	Most Acidic	(1) ACD
pKa (PKA)	7.56+/-0.40	Most Basic	(1) ACD
Vapor Pressure (VP)	3.88E-11 Torr	25.0 deg C	(1) ACD

(1) Calculated using Advanced Chemistry Development (ACD/Labs) Software
Solaris V4.67 ((C) 1994-2004 ACD/Labs)

See HELP PROPERTIES for information about property data sources in REGISTRY.

213 REFERENCES IN FILE CA (1907 TO DATE)
7 REFERENCES TO NON-SPECIFIC DERIVATIVES IN FILE CA
215 REFERENCES IN FILE CAPLUS (1907 TO DATE)

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